Chemistry 110A – Physical Chemistry: Introduction to Quantum Mechanics, Spring 2023

Instructor:Chenchen Song (ccsong@ucdavis.edu)Lectures:MWF 10:00 – 10:50 AM, TLC 1218TA and Contact Info:

A01 Heejune Park (heepark@ucdavis.edu)

Discussion R 6:10–7:00 PM, Wellman 7

Office hours:

Chenchen Song, Wednesday 1-2PM, Chemistry 190B

Heejune Park, Tuesday 10-11AM, Chemistry, 190A

Course Webpage: Accessible through Canvas to registered students. **Course Materials:**

- McQuarrie and Simon, <u>Physical Chemistry: A Molecular Approach.</u> This textbook is a classic and used by 110A students for many years; Donald McQuarrie was a Chemistry professor at UC Davis in the years of 1978–1994.
- Optional: Cox, Problems and Solutions to accompany Physical Chemistry: A Molecular Approach.

How to obtain: If you are enrolled in Equitable Access, you can access the textbook by clicking "Bookshelf" on Canvas. During the quarter, you will be able to download the textbook using the Bookshelf app, which will give you access to the digital textbook that does not expire.

If you are not enrolled in Equitable Access, physical copies of the textbook are available at <u>uscibooks.aip.org</u> and digital copies are available for rent and purchase from <u>www.redshelf.com</u>.

Additional readings may be provided in the form of PDFs uploaded to Canvas.

Prerequisites: Preparation in <u>multivariable calculus</u>, <u>differential equations</u>, <u>linear algebra</u>, <u>complex numbers</u> and the <u>classical physics of particles and waves</u> is needed to succeed in this course. <u>If you have not completed these prerequisites</u>, this course will not be a good fit for you. We will not have time for extensive review of these topics. The formal prerequisites are:

- CHE 2C or 2CH (one year of general chemistry).
- PHY 7C, 9C or 9HC (one year of classical physics).
- MAT 16C, 17C, or 21C (one year of calculus with basic differential equations).

In addition, you are highly recommended to have taken MAT 021D (multivariable calculus & vector analysis), MAT 022A / 22AL (linear algebra with computational lab), and MAT 22B (differential equations) prior to this course.

Lecture attendance: Lecture attendance is encouraged but not required. You will have opportunities to earn extra participation credits. There is no penalty for not attending lecture, but attendance is required during exam periods (see Exams).

Lecture recordings: Our classroom is "lecture-capture enabled": audio and slides will be recorded, but boardworks cannot be recorded. The recordings will be available on Canvas. According to the instruction I received:

"Links to the recorded lectures will typically appear on your Canvas course site within an hour or two of the end of each class. The videos will appear in "Lecture Videos" and/or "Media Gallery" in the course navigation section of your Canvas course site. We will enable these sections on your site shortly before the start of the quarter."

Extra participation points through iClicker: Current plan for extra participation credit questions in lecture is to use the iClicker student app on your phone or tablet. You can register an iClicker account using your ucdavis email. For detailed instructions, please visit the site <u>here</u> and see instructions under "student documentations".

Discussion: Each TA will lead one discussion section, starting the first week. The content and format of discussion sections is up to the individual TA.

Office Hours: Office hours will start the second week.

Problem Sets: <u>There are 7 problem sets</u>. <u>The lowest problem set grade will be dropped</u>. Problem sets will generally be posted on or before Monday, and due by the end of the following Monday. (see Important Dates).

For electronic submissions, please submit to Canvas. Please do not submit through emails as they may get lost.

For physical submissions, please drop off at TA's mailboxes (located on the first floor of the Chemistry building).

Late problem sets will be accepted until the end of Friday, with a reduced grade of 10% per day late. The reduction in the problem set grade is applied as a percentage taken off points earned. For example, an assignment turned on Thursday (two days late) and graded as 60 points will have 20% of 60 points (i.e. 12 points) taken off for lateness.

Regrade requests for problem sets: You can pick up your homework from the TA during the discussion section or the TA's office hour. If you would like to submit a regrade request, please send an email to your TA within two weeks from the date when you receive a grade on Canvas. In your email, please include the following information: (a) A photo of the related page of your homework, (b) describing which part of the photo needs a regrade, and (c) a brief explanation on why you think a regrade is necessary.

Examinations: There will be <u>one midterm and one cumulative final exam</u> (see <u>Important Dates</u>). Midterm will be during the normal lecture time in the classroom. The final exam will be <u>June, 15</u> <u>10:30 AM</u> and two hours in length. <u>Both exams are in-person and open book</u>. You can refer to any physical notes and books during the exam. You can also use electronic devices to view any local files, but internet connection is not allowed during the exam.

Taking the exam early requires prior approval of the instructor. There are no makeup exams. Accommodations for exams will be granted with a letter from the Student Disability Center.

Grading: The point distribution for the course is as follows:

1) If the percentage score of your final is higher than your midterm:

Problem sets 40%, Midterm 15%, Final 45%

2) If the percentage score of your midterm is higher than your final:

Problem sets 40%, Midterm 30%, Final 30%

Letter grades will be assigned according to the following scale: A– to A+, 85% - 100%; B– to B+, 70% - 84%; C– to C+, 60% - 69%; D– to D+, 50% - 59%. You may request an incomplete grade

if you have completed the majority of the course and are currently passing but cannot complete the course; we will handle these on a case-by-case basis.

Adding/Dropping, Pass/No Pass, Cancellation/Withdrawal: Last day to add or drop the course with a PTA / PTD (Permission to Add / Drop) number, to opt in or out of P/NP grading, to submit cancellation/withdrawal form is June 8.

Important Dates:

| | М | Т | W | Th | F |
|---------------|--------------|------------|------------|----|------------|
| Week 1 (4/3) | Lecture 1 | | Lecture 2 | | Lecture 3 |
| Week 2 (4/10) | Lecture 4 | | Lecture 5 | | Lecture 6 |
| | PS1 posted | | | | |
| Week 3 (4/17) | Lecture 7 | PS1 due | Lecture 8 | | Lecture 9 |
| | PS2 posted | | | | |
| Week 4 (4/24) | Lecture 10 | PS2 due | Lecture 11 | | Lecture 12 |
| | PS3 posted | | | | |
| Week 5 (5/1) | Lecture 13 | PS3 due | Lecture 14 | | Lecture 15 |
| | PS4 posted | | | | |
| Week 6 (5/8) | Lecture 16 | PS4 due | Lecture 17 | | Midterm |
| | | | | | |
| Week 7 (5/15) | Lecture 18 | | Lecture 19 | | Lecture 20 |
| | PS5 posted | | | | |
| Week 8 (5/22) | Lecture 21 | PS5 due | Lecture 22 | | Lecture 23 |
| | PS6 posted | | | | |
| Week 9 (5/29) | Memorial Day | PS7 posted | Lecture 24 | | Lecture 25 |
| | | PS6 due | | | |
| Week 10 (6/5) | Lecture 26 | | Lecture 27 | | |
| | | | PS7 due | | |

Final exam: June, 15 10:30 AM-12:30PM

Learning Goals: We will introduce the conceptual and mathematical foundations of quantum mechanics, key model problems and examples, applications to atoms and diatomic molecules, and approximate methods. Topics are listed in rough chronological order:

Topic

<u>Textbook chapter</u>

| 1. | Experiments show the need for a quantum theory | 1 and supplement |
|----|---|--------------------|
| 2. | Classical waves: Traveling and standing waves, superposition and inter- | ference 2 |
| | Review of complex numbers | MathChapter A |
| | The quantum mechanical wavefunction: General concepts | 4.1 and supplement |
| | Review of probability and statistics | MathChapter B |
| 3. | Time-independent Schrödinger's Equation and particle in a box | 3 |
| 4. | Conceptual foundations of quantum mechanics: | 4 |
| | Postulates, wavefunctions, normalization, Hermitian operators, eigenfun | nctions and |
| | expectation values, time dependence; uncertainty principle and commut | |
| 5. | Models of molecular vibration and rotation: | 5 |
| | The harmonic oscillator and rigid rotor | |
| 6. | Quantum mechanics of the hydrogen atom: | 6 |
| | Separation of variables, quantum numbers, | |
| | and visualization of wavefunctions | |

| 7. | Approximations: Variational method and perturbation theory | 7 |
|----|--|---|
| 8. | Multielectron atoms: Identical particles, wavefunction antisymmetry, | 8 |
| | electron spin, Slater determinants, Hartree-Fock method, atomic term symbols | |
| 9. | Diatomic molecules: Molecular orbital theory, | 9 |
| | bonding and antibonding orbitals, and molecular term symbols | |

Additional Materials:

The <u>Feynman Lectures on Physics</u> is a wonderful resource and made freely available by CalTech. In particular, Volume III on quantum mechanics is especially relevant to this course. Some excerpts from this book will be used as supplemental material.

The <u>HyperPhysics</u> website, hosted by the Department of Physics and Astronomy at Georgia State, contains valuable online resources on quantum mechanics.

Note on Copyright: The following language is included to clarify what you are legally allowed to do with digital course materials.

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Academic Honesty: You are expected to follow the <u>Code of Academic Conduct</u>. Collaborating on problem sets is allowed in the spirit of students helping one another understand the material, and each student needs to turn in independent solutions that reflect their own understanding. Examples of activities not allowed that may result in a SJA referral include: Copying solutions to problem sets; collaboration on exams; and getting help from "tutoring" websites such as chegg or coursehero, either by submitting questions / content or searching for existing answers. We do not enjoy making SJA referrals at all – it is time-consuming and stressful to all involved – so please be fair to your classmates and uphold the high standards that we expect from UC Davis students.